

Absorption spectrum of the mixed valence Cr³⁺-Cr²⁺ pair center in KZnF₃ crystal

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Abstract

Assignment of absorption lines of mixed valence Cr³⁺-Cr²⁺ pair center has been done by the analysis of the probabilities of exchange-induced electric-dipole transitions. Parameters of exchange interaction $J_1 = 44.5 \pm 5 \text{ cm}^{-1}$ and axial crystal field $B_2^0 = -19.6 \pm 2 \text{ cm}^{-1}$ for the excited state $|Cr^{2+}3E_g; Cr^{3+}4A_2\rangle$ have been estimated from the fine structure of absorption spectra of the pair. Using microscopic theory of superexchange interaction for the ground and excited states of the pair the value of the transfer integral of eg-electron via the intermediate fluorine ion $t_{vv} = 3500 \text{ cm}^{-1}$ has been extracted.

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Keywords

Double exchange, Exchange interaction, Mixed valence, Optical spectroscopy